consecutive hybrid quadruplexes. With addition of crowding mimetics (Ficoll 70; Ficoll 400; and PEG 200 (20 and 40% w/v)) to the HT4 sequence, CD studies show a conformational switch to an antiparallel structure in Ficoll 400 (40% w/v) and a parallel conformation in PEG 200 (40% w/v), with no conformational changes observed in Ficoll 70. For HT8, a similar effect was observed, but in addition an anti-parallel conformation was obtained in Ficoll 70 (40% w/v), which suggests an enhanced sensitivity to dehydration for the HT8 sequence. Additionally, thermal CD melting studies showed stabilization of HT8 conformation in Ficoll compared with HT4. With binding of NMM to HT4 in 20% (w/v) crowding mimetics a shift to the parallel conformation was observed. However, the antiparallel (more dehydrated) conformation for HT8 is promoted in Ficoll 400. We plan more detailed environmental studies of NMM binding to qDNA under crowding conditions using fluorescence spectroscopy.
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Zipper Like Structures Possible Intermediates to Assemble Duplex Mediated G-Quadruplex DNA
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In this paper we report the detailed characterization at the atomic level by molecular mechanics of Guanine-rich DNA that forms zipper-like structures. These duplexes in vitro have shown to associate into G-quadruplex that are conformed by two duplexes. We want to known at the atomic level how the association process works, but the structure of the duplex for these sequences has not been established. This is a preliminary work to be able to model the formation of the zipper structure (G-quadruplex mediated structure). Such process has been hypothesized to work at sites rich in Gs and be involved in process like meiosis, pairing homologues chromosomes and the structural function of telomeres. Models were constructed and these structures minimized and equilibrated, allowing analysis via molecular dynamics to understand the factors that determines the most stable structure. Preliminary analysis studying the intrinsic chemical stability showed that the presence of positively charged ions near the Gs-rich region of the studied sequences is critical to the stability of these DNA structures. It has been shown that simulating divalent cations can be challenging and that the force fields have to be tested for non canonical DNA conformations. This particular structure has a normal close to B-DNA section but the ''zipper-like'' is definitively a region that needs to be carefully studied to check the adequacy of the modeling tools used. The dynamics of these molecules show us that zipper structures have more stability with sodium ions in simulated conditions. In summary, the results allow a better understanding of this system at the molecular level, allowing us to predict the likelihood of formation of these structures in vivo as well the features of the sequences that could fold as zipper-like structures.

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Existence and Possible Function of Buckled DNA in Tailed DSDNA Bacteriophage Portals
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Tailed double-stranded DNA (dsDNA) bacteriophages control genome packaging and ejection from their viral capsids using a portal system. The portal vertex serves as a docking site for the viral ATPase packing motor which translocates DNA through the central channel during packaging. In the case of several well-studied bacteriophages including T7 and ε15, the central channel extends into the capsids interior by a core assembly of stacked, cylindrical protein subunits. Often possessing different internal diameters, these protein subunits can create large cavities in an otherwise straight channel. The height of these cavities are typically within 10-20% of the DNA persistence length and, in the case of T7, the cavity is 50Å tall and 110Å wide. Given that these cavities exist upstream of the packing motor, we postulate that they allow DNA to buckle under large packing forces (~100 pN). A cryo-EM reconstruction of φ29 revealed that DNA buckles in a toroidal supercoil within a cavity only 3.5 times wider and 2.5 times taller than the width of DNA. A recent reconstruction of bacteriophage P22 also revealed DNA density inside its portal cavity that is over twice the width of dsDNA, suggesting that DNA may be compressed into a highly-bent supercoil. using analytic and numerical approaches, we compute the forces required for and during DNA buckling in bacteriophages T7 and P22. We demonstrate that DNA can indeed buckle and that the buckled conformation subsequently pushes outward on the cavity. Thus, the buckle could mechanically initiate a conformational change in the portal protein to provide the head-full signal.

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Coarse-Grained Model DNA with Explicit H-Bonding and Implicit Solvent
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We present a coarse-grained model for DNA that is intended to function realistically at the level of individual bases. The model is composed of residues with up to eight coarse-grained beads each, which is sufficient for DNA-like base stacking and base-base recognition by hydrogen bonding. The beads interact by means of short-ranged pair potentials and a simple implicit solvent model. Movement is simulated by Brownian dynamics without hydrodynamic coupling. The main stabilizing forces are base stacking and hydrogen bonding, as modified by the effects of solvation. Complementary double-stranded chains of such residues form stable double helices over long runs (~10 μs) at or near room temperature, with structural parameters close to those of B-form DNA. Most mismatched chains or mismatched regions within a complementary molecule melt and become disordered. Long-range fluctuations and elastic properties, as measured by bending and twisting persistence lengths, are close to experimental values. Single-stranded chains are flexible, with transient stretches of free bases in equilibrium with globules stabilized by intrastrand stacking and hydrogen bonding. Model DNAs in covalently closed loops form right or left-handed supercoils, depending on the sign of overtwist or undertwist. Short stem-loop structures melt at elevated temperatures and reanneal when the temperature is carefully lowered. Overall, most qualitative properties of real DNA arise naturally in the model from local interactions at the base pair level.

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Molecular Dynamics Study of Cobalt(III) Hexammine Counter-Ion Distributions around B-DNA and A-RNA Duplexes
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Multivalent ions are known to induce strong attractive forces between DNA strands resulting in DNA condensation. At the same time, short double-stranded (ds) RNA helices resist condensation by trivalent Cobalt hexammine (Cohex) in the DNA condensing ionic conditions. To explore the factors that could lead to this difference in condensation, we have carried out a set of explicit solvent molecular dynamics simulations of 25 base pairs canonical B-DNA and A-RNA duplexes under different salt conditions. Several mixtures of monovalent (Na, Cl) and trivalent (Cohex) ions are considered. The results of simulation show that Co-hex ions effectively displace monovalent Na ions from the major groove of dsRNA binding to the RNA phosphate oxygens. The ions are buried within the major groove with a distribution peak at 7.3 Angstrom from the helix axis. their density rapidly decreases and becomes negligible at 11 A from the axis. In contrast to that, the distribution of Cohex around B-DNA is shifted outside the helix with a peak at 13.3 A from the helix axis. The ions prefer to bind to the phosphate groups on the outer surface of B-DNA. The observed difference in Cohex distributions around B-DNA and A-RNA is in agreement with the proposed explanation of the resistance of RNA to condensation due to a difference in Cohex binding to DNA and RNA (L.Li et al., PRL 106, 108101 (2011)).

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Dynamic NMR Studies Provide Insight into Sequence Dependent Binding Affinities
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The ability of molecules to bind DNA plays an important role in many biological processes including, transcription, regulation, replication, repair. Understanding the factors that influence binding affinity is therefore essential to our understanding of these processes.